Exploration on DNA binding ability of heteroleptic ligand metal complexes: Synthesis and characterization

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Abstract - Two heteroleptic ligand metallointercalators (Cu(II) and Zn(II)) have been synthesized using Knoevenagel condensate β-diketone ligand (obtained by the condensation of acetylacetone and cinnamaldehyde) as primary ligand and 1,10-phenanthroline as co-ligand in order to find out whether there is an enhancement in the efficacy of biological activities. They have been characterized by elemental analysis, magnetic susceptibility, molar conductance measurements, UV-Vis., FT IR and ^{13}NMR spectral studies. These complexes show higher molar conductance values, supporting their electrolytic nature. Spectroscopic and other analytical data of the complexes suggest square planar geometry around the central metal ion. The binding properties of these complexes with DNA have been explored by electronic absorption spectra. It reveals that the complexes have the ability to interact with calf thymus DNA (CT DNA) by intercalative mode. The binding constant values (Kb) clearly signify that the copper(II) complex have more intercalating ability than zinc(II) complex. The *in vitro* antibacterial and antifungal assay indicates that these complexes are good antimicrobial agents against various pathogens. It has been investigated by Minimum Inhibitory Concentration (MIC) method.

Keywords:

1. INTRODUCTION

Several ligands derived from β-diketones are also known to form metal complexes. These ligands derived from β-diketones have been employed for the preparation of new complexes. The β-diketone ligands are considered as potential ligands due to their enolising ability. β-diketone and its metal complexes have been widely used in diverse areas because of their unique structural features, chemical functionalities, and toughness for light and heat as electroluminescence materials [1]. β-diketone derivatives possess a broad spectrum of biological effects such as antiinflammatory and antimicrobial activity effects [2,3]. But being incapable of enolisation, the condensates have not perhaps been considered earlier as potential ligands towards transition metal ions.

Nowadays, special attention has been paid for the synthesis of effective conjugative and versatile chelating systems with metal ions due to their novel structural features, unusual redox behaviour and relevance to biological processes [4]. Amongst various systems, the coumpounds derived from Knoevenagel condensate ligand have gained much interest due to their delocalized π-orbitals, flexible behaviour, multifunctional ligand sites *etc*. In order to form the higher degree of conjugated versatile ligand system, Knoevenagel condensate ligand is designed for the formation of stable complexes. Studies of these structure, spectral and redox properties would be optimum models for the metalloproteins, which are essential to address the structure–redox relationship [5].

Keeping the facts in mind, herein the synthesis and characterization of Cu(II) and Zn(II) metal complexes containing Knoevenagal condensate ligand and 1,10-phenanthroline (heteroleptic ligand complexes) are described. These complexes have been characterized by physicochemical and various spectral techniques. Their DNA binding analysis has been carried out *via* electronic absorption titration method. Further, all the synthesized compounds were screened for their *in vitro* antimicrobial activity against various bacterial and fungal strains.

2. EXPERIMENTAL PROTOCOLS

2.1 Materials and Methods

The chemicals involved in this work were of AnalaR grade and were used without further purification. However, the solvents were purified by the standard procedure. Acetylacetone, cinnmaldehyde and 1,10-